



Argonne Training Program on Extreme-Scale Computing

Introduction to ATPESC

Ray Loy
ATPESC 2020 Program Director

Thanks to Marta Garcia, ATPESC 2016-2019 Program Director



Outline

 **Welcome**

 **Argonne National Laboratory**

 **ATPESC Overview**

 **Logistics**

 **Tour(?)**

Welcome!

73 ATPESC 2020 Participants

Alan	Albert	Alberto	Aleksandra	Amanda	Amil
Ana	Antonin	Ashka	Bruce	Carlos	Choah
Denis	Derek	Dmitry	Dossay	Dylan	Eremey
Evan	Francois	Georgios	Giuseppe	Henry	Hugo
Ian	Igor	Imanuel	Jacob	Jared	Jeremy
Jorge Luis	Joseph	Juan Diego	Justin	Kento	Kevin
Komal	Kyle	Ligia Diana	Łukasz	Maciej	Malik
Massimiliano	Matthew	Md Fazlay	Melisa	Michael	Michael
Michelle	Ming	Muaaz	Muhong	Mukund	Nathan
Nathaniel	Neil	Neil	Niels	Patrick	Philippe
Ral	S M	Soonpil	Steven	Suyash	Thomas
Valeria	Victor	Yangzesheng	Yiban	Zac	Zhi
Zongcai					

Welcome!

ATPESC 2020

45 Institutions

Argonne National Laboratory
CEA Saclay
Canadian Nuclear Laboratories
Colorado State University
Cornell University
Iowa State University
LUT University
Lawrence Livermore National Laboratory
Michigan State University
NASA Langley Research Center
National Renewable Energy Laboratory
Naval Surface Warfare Center
Oak Ridge National Laboratory
Princeton Plasma Physics Laboratory
Rensselaer Polytechnic Institute
Stanford University
The Australian National University
University of Colorado Boulder
University of Illinois at Urbana-Champaign
University of Minnesota
University of Saskatchewan
University of Tennessee
Westinghouse Electric Company, LLC

BP
CU Boulder
Carnegie Mellon University
Columbia University
Environment and Climate Change Canada
KTH Royal Institute of Technology
Lawrence Berkeley National Laboratory
Los Alamos National Laboratory
NASA Ames Research Center
NERSC
Naval Postgraduate School
Numerical Algorithms Group (NAG)
Oregon State University
Purdue University
Sandia National Lab
Texas A&M University
University of Chicago
University of Florida
University of Michigan
University of Notre Dame
University of Southern California
University of Warsaw

Argonne National Laboratory

Argonne – a part of DOE National Laboratory System

Office of Science Laboratories

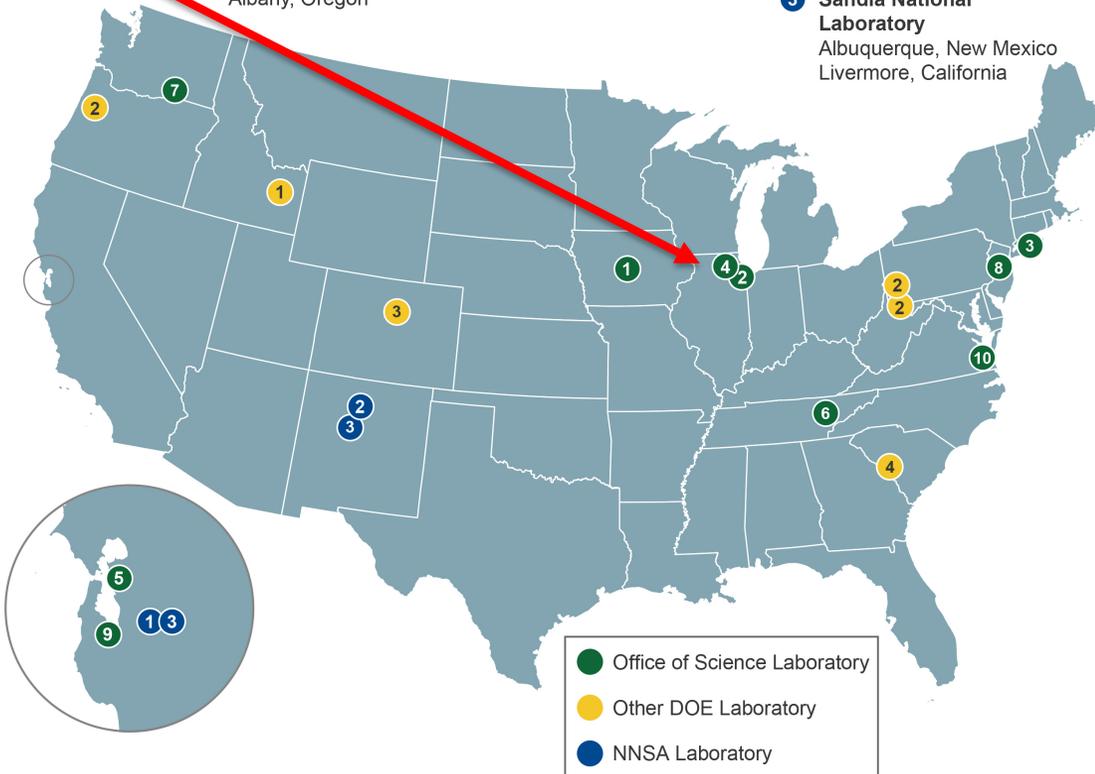
- 1 Ames Laboratory
Ames, Iowa
- 2 Argonne National Laboratory
Argonne, Illinois
- 3 Brookhaven National Laboratory
Upton, New York
- 4 Fermi National Accelerator Laboratory
Batavia, Illinois
- 5 Lawrence Berkeley National Laboratory
Berkeley, California
- 6 Oak Ridge National Laboratory
Oak Ridge, Tennessee
- 7 Pacific Northwest National Laboratory
Richland, Washington
- 8 Princeton Plasma Physics Laboratory
Princeton, New Jersey
- 9 SLAC National Accelerator Laboratory
Menlo Park, California
- 10 Thomas Jefferson National Accelerator Facility
Newport News, Virginia

Other DOE Laboratories

- | | |
|--|---|
| 1 Idaho National Laboratory
Idaho Falls, Idaho | 3 National Renewable Energy Laboratory
Golden, Colorado |
| 2 National Energy Technology Laboratory
Morgantown, West Virginia
Pittsburgh, Pennsylvania
Albany, Oregon | 4 Savannah River National Laboratory
Aiken, South Carolina |

NNSA Laboratories

- 1 Lawrence Livermore National Laboratory
Livermore, California
- 2 Los Alamos National Laboratory
Los Alamos, New Mexico
- 3 Sandia National Laboratory
Albuquerque, New Mexico
Livermore, California



Together, the **17 DOE laboratories** comprise a preeminent federal research system, providing the Nation with strategic scientific and technological capabilities. The laboratories:

- Execute long-term government scientific and technological missions, often with complex security, safety, project management, or other operational challenges;
- Develop unique, often multidisciplinary, scientific capabilities beyond the scope of academic and industrial institutions, to benefit the Nation's researchers and national strategic priorities; and
- Develop and sustain critical scientific and technical capabilities to which the government requires assured access.

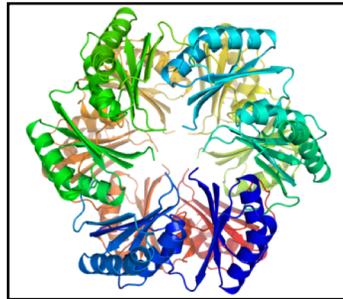
Source: https://science.energy.gov/~media/ /images/laboratories/DOE_Laboratories_Map_2014_Hi-res.jpg



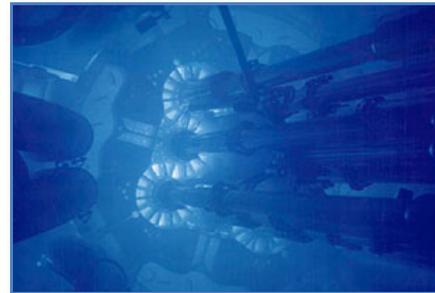
Argonne's mission: Provide science-based solutions to pressing global challenges



Energy Science



Environmental Sustainability

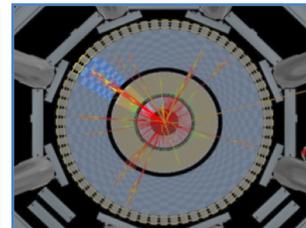
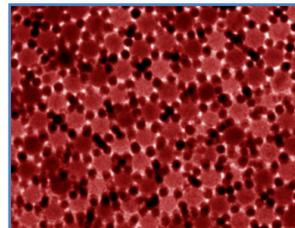


Nuclear and National Security

*Use-Inspired Science and Engineering ...
... Discovery and transformational Science and Engineering*



Major User Facilities



Science and Technology Programs

RESEARCH DIVISIONS

Computing, Environment and Life Sciences

BIO	Biosciences
EVS	Environmental Science
MCS	Mathematics and Computer Science

Energy and Global Security

ES	Energy Systems
GSS	Global Security Sciences
NE	Nuclear Engineering

Photon Sciences

ASD	Accelerator Systems
AES	APS Engineering Support
XSD	X-ray Science

Physical Sciences and Engineering

CSE	Chemical Sciences and Engineering
HEP	High Energy Physics
MSD	Materials Science
NST	Nanoscience and Technology
PHY	Physics

FACILITIES, CENTERS, AND INSTITUTES

User Facilities

APS	Advanced Photon Source
ALCF	Argonne Leadership Computing Facility
ATLAS	Argonne Tandem Linear Accelerator System
ARM	ARM Southern Great Plains
CNM	Center for Nanoscale Materials

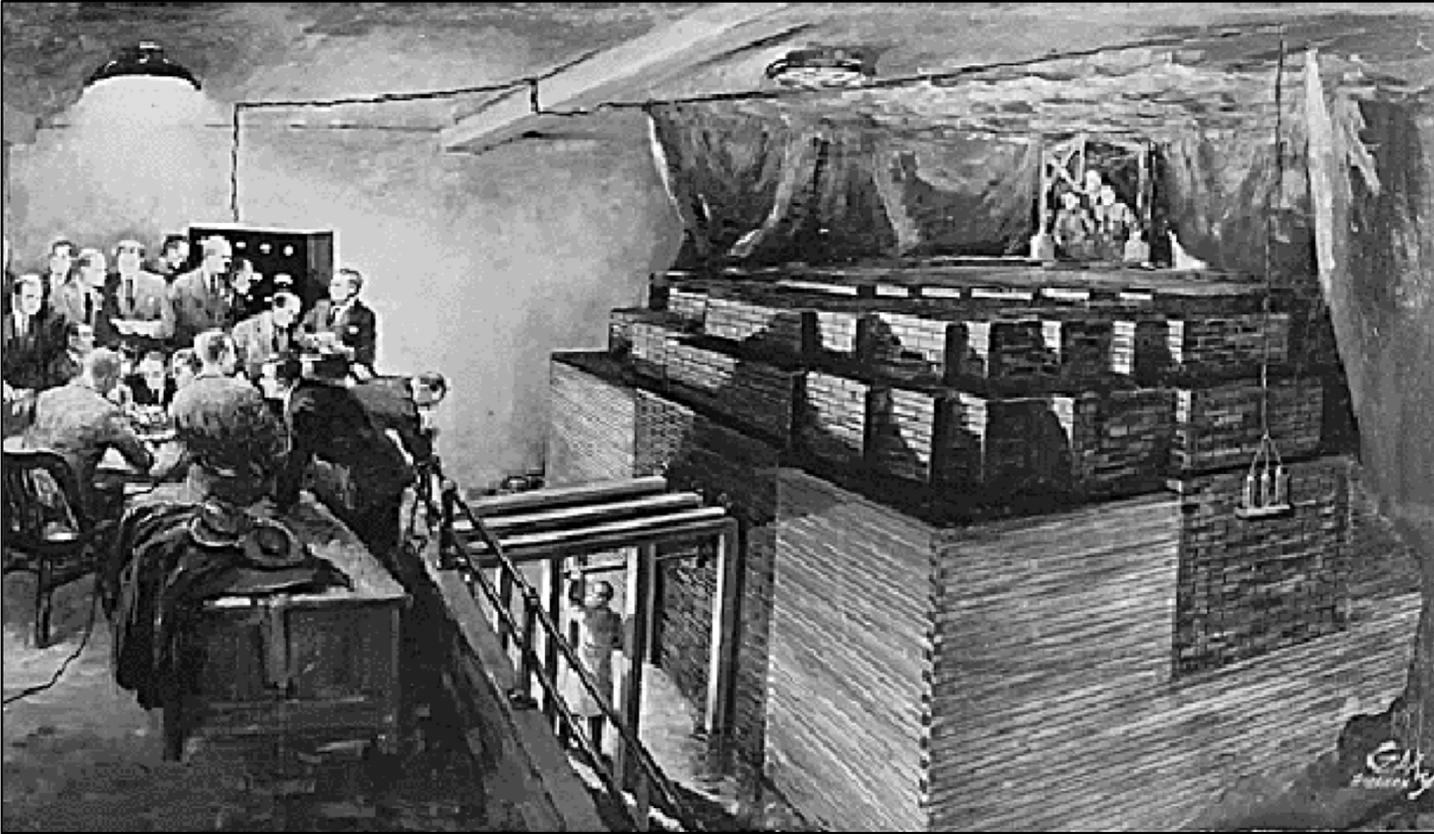
Centers and Joint Institutes

AAI	Argonne Accelerator Institute
ACCESS	Argonne Collaborative Center for Energy Storage Science
ADW	Argonne Design Works
ALI	Argonne Leadership Institute
CEES	Center for Electrochemical Energy Science
CTR	Center for Transportation Research
CRI	Chain Reaction Innovations
CI	Computation Institute
IACT	Institute for Atom-Efficient Chemical Transformations
IGSB	Institute for Genomics and Systems Biology
IME	Institute for Molecular Engineering
JCESR	Joint Center for Energy Storage Research
MCSG	Midwest Center for Structural Genomics
NSP	National Security Programs
NAISE	Northwestern-Argonne Institute for Science and Engineering
RISC	Risk and Infrastructure Science Center
SBC	Structural Biology Center

<https://www.anl.gov>

The origin of Argonne National Laboratory

CP-1 under the bleachers of Stagg field at U. Chicago



Chicago Pile-1 was the world's first artificial nuclear reactor. The first man-made self-sustaining nuclear chain reaction was initiated on December 2, 1942



Chicago Pile-1: A Brick History

<https://www.youtube.com/watch?v=mTPiTJ2bKS0>

Aerial view of Argonne National Laboratory

Advanced
Photon
Source
(APS)

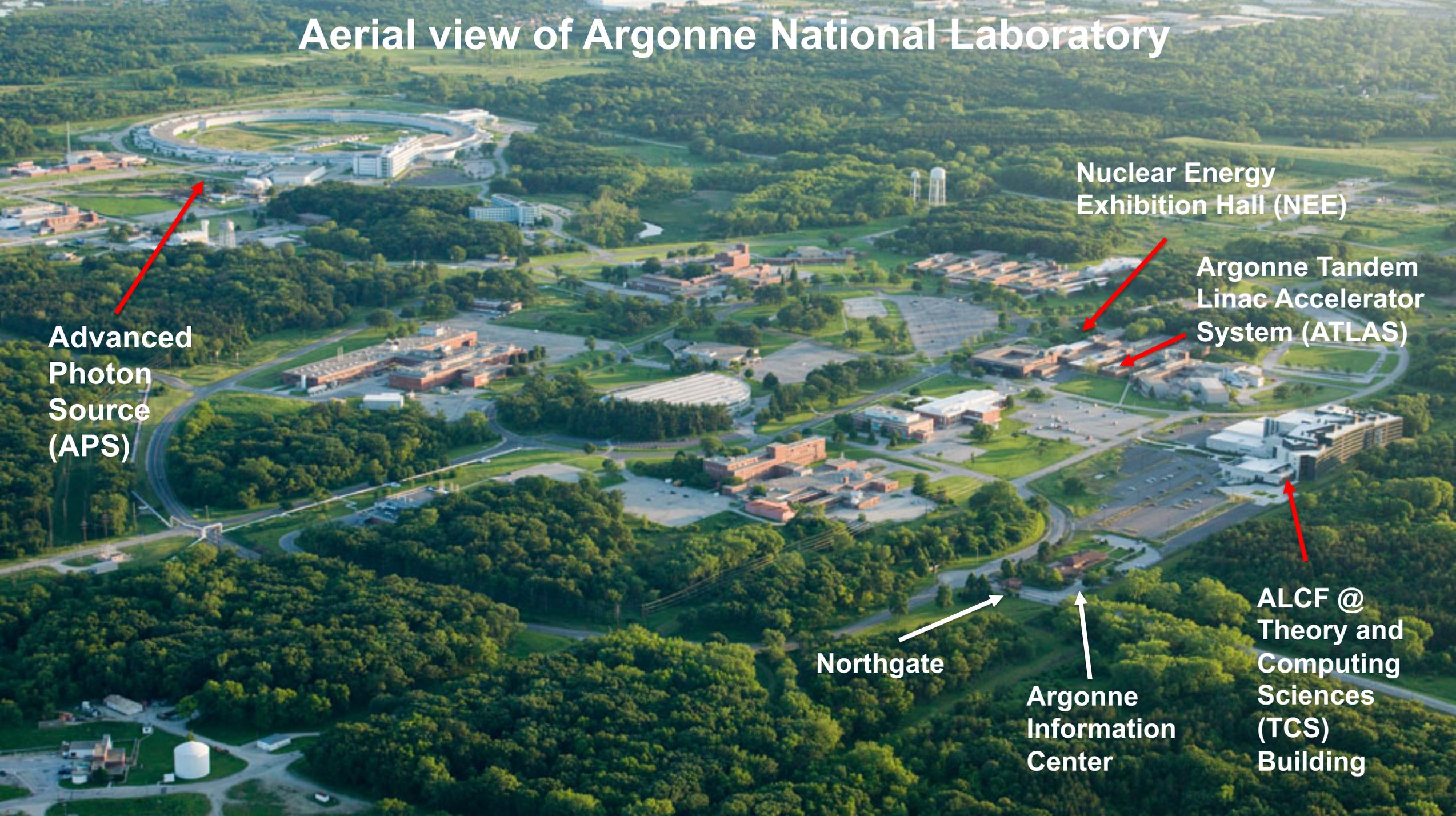
Nuclear Energy
Exhibition Hall (NEE)

Argonne Tandem
Linac Accelerator
System (ATLAS)

ALCF @
Theory and
Computing
Sciences
(TCS)
Building

Northgate

Argonne
Information
Center

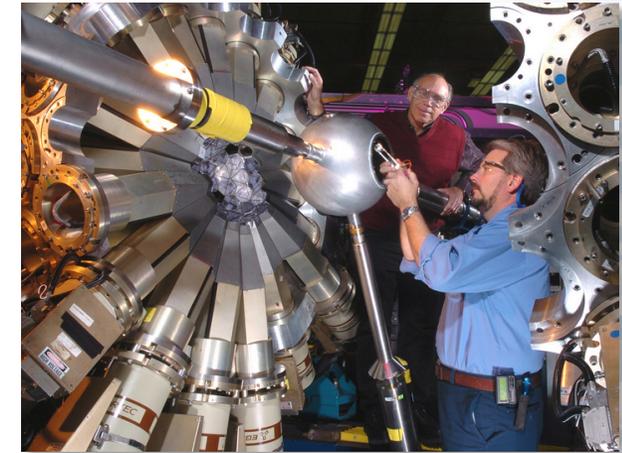


Major Scientific User Facilities at Argonne

Advanced Photon Source



Argonne Tandem Linear Accelerator System



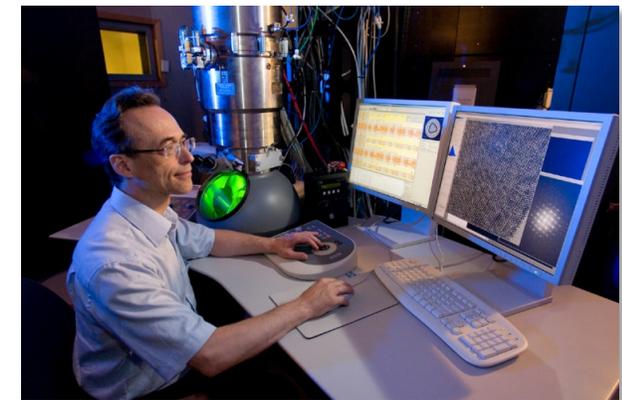
Center for Nanoscale Materials



Argonne Leadership Computing Facility

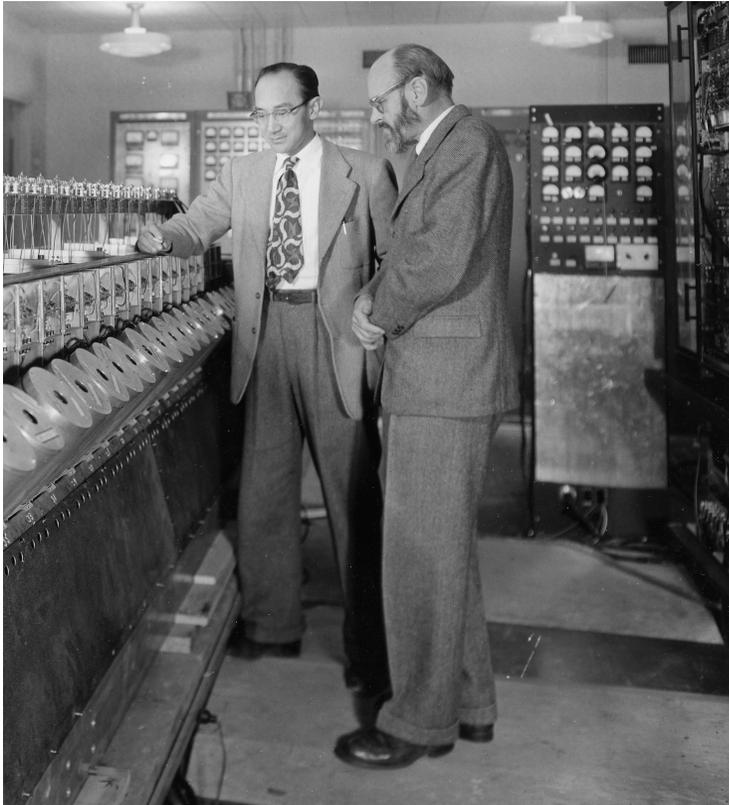


Electron Microscopy Center



AVIDAC (1949-1953)

Argonne's Version of the Institute's Digital Arithmetic Computer



“Moll” Flanders, Director
Jeffrey Chu, Chief Engineer

- **AVIDAC:** based on a prototype at the Institute for Advanced Study in Princeton
- **Margaret Butler wrote AVIDAC's interpretive floating-point arithmetic system**
 - Memory access time: 15 microsec
 - Addition: 10 microsec
 - Multiplication: 1 millisecc
- **AVIDAC press release:**
100,000 times as fast as a trained “Computer” using a desk calculator

Early work on computer architecture



Margaret Butler helped assemble the ORACLE computer with ORNL Engineer Rudolph Klein

In 1953...

ORACLE was the world's fastest computer, multiplying 12-digit numbers in .0005 seconds (2Kop/s).

Designed at Argonne, it was constructed at Oak Ridge.

The future... Aurora Exascale System



Motivation for ATPESC

- Today's most **powerful supercomputers** have **complex hardware architectures** and **software environments**
 - and even greater complexity is on the horizon on next-generation and exascale systems
- The **scientific and engineering applications** developed for these systems are themselves **complex**
- There is a **critical need for specialized, in-depth training for the computational scientists** poised to facilitate breakthrough science and engineering using these systems

ATPESC Overview

- Founded by Paul Messina in 2013
- Conceived as a 2-week retreat
- Renowned computer scientists and HPC experts from US national laboratories, universities, and industry serve as lecturers and guide hands-on sessions.
- Target audience: advanced doctoral students, postdocs, and early career computational scientists
- No fee to participate. Domestic travel, meals, and lodging provided.
- Competitive application process reviewed by committee
 - Must have experience with MPI and/or OpenMP
 - Experience with at least one HPC system
 - Concrete plans to conduct CSE research on large-scale computers

Curriculum Tracks and their leaders

- **Track 1: Hardware Architectures** – Pete Beckman
- **Track 2: Programming Models and Languages** – Rajeev Thakur and Yanfei Guo
- **Track 3: Data-intensive Computing and I/O** – Rob Latham and Phil Carns
- **Track 4: Visualization and Data Analysis** – Mike Papka, Joseph Insley, and Silvio Rizzi
- **Track 5: Numerical Algorithms and Software for Extreme-Scale Science** – Lois McInnes, Mark Miller, and Alp Dener
- **Track 6: Performance Tools and Debuggers**– JaeHyuk Kwack and Scott Parker
- **Track 7: Software Engineering** – Anshu Dubey and Katherine Riley
- **Track 8: Machine Learning and Deep Learning for Science** – Venkatram Vishwanath

ATPESC Computing Resources

The screenshot shows the 'User Facilities at a Glance' page for ASCR User Facilities. The page header includes 'SC Home Organization Jobs Contact' and 'DOE Home'. The main navigation bar lists 'Programs', 'Laboratories', 'User Facilities', 'Universities', 'Funding Opportunities', 'News', and 'About'. The breadcrumb trail reads 'You are here: SC Home » User Facilities » User Facilities at a Glance » ASCR User Facilities'. The page title is 'User Facilities' and the sub-header is 'User Facilities at a Glance ASCR User Facilities'. A sidebar on the left contains links for 'All User Facilities', 'ASCR User Facilities', 'BES User Facilities', 'BER User Facilities', 'FES User Facilities', 'HEP User Facilities', 'NP User Facilities', 'User Resources', 'User Statistics', 'Policies and Processes', 'Frequently Asked Questions', 'User Facility Science Highlights', and 'User Facility News'. The main content area features a 'CONTACT INFORMATION' box for the Office of Science and four facility descriptions, each with a photo and a brief description: Argonne Leadership Computing Facility (ALCF), Energy Sciences Network (ESnet), National Energy Research Scientific Computing Center (NERSC), and Oak Ridge Leadership Computing Facility (OLCF).

 **ALCF** – Theta and Cooley

 **OLCF** - Ascent

 **NERSC** – Cori et al.

 **Intel Devcloud**

Source: <https://science.energy.gov/user-facilities/user-facilities-at-a-glance/ascr/>

Goals for Attendees



Exposure to New ideas



Take advantage of ATPESC Resources



Talk F2F (virtually) with Lecturers, other Participants, Support

Argonne NATIONAL LABORATORY

HOME ATPESC NEWS ABOUT ATPESC PAST PROGRAMS

Agenda 2020

[[Introductions](#) | [Track 1](#) | [Track 2](#) | [Track 3](#) | [Track 4](#) | [Track 5](#) | [Track 6](#) | [Track 7](#) | [Track 8](#)]

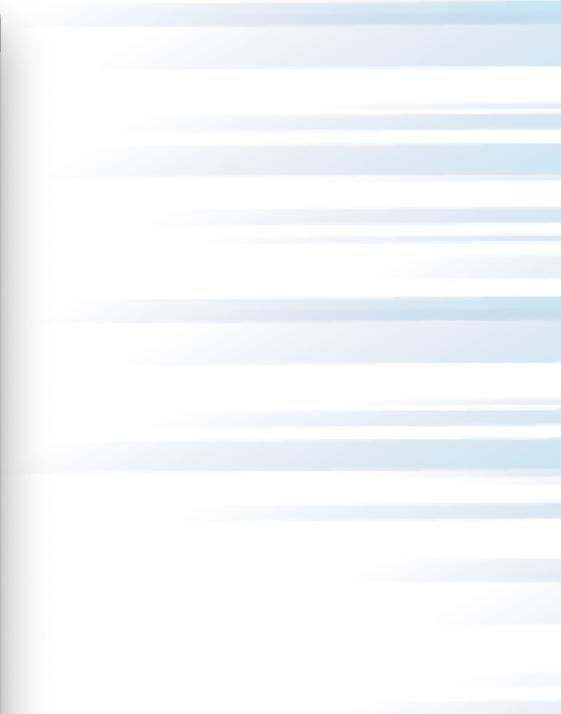
ALL TIMES ARE U.S. CENTRAL DAYLIGHT TIME (UTC-5)
[MEETING CONNECTION INFO AND HANDOUTS](#)

SUNDAY, July 26, 2020

11:00	Introduction to ATPESC	Ray Loy, ANL
11:30	Quick Start on ATPESC Computing Resources	JaeHyuk Kwack, ANL
1:00 p.m.	Participant Introductions	All
2:00	Adjourn	

MONDAY, July 27, 2020

X Highlight All Match Case Match Diacritics Whole Words



The screenshot shows a web browser window displaying the Argonne National Laboratory Box file manager. The address bar shows the URL `anl.app.box.com/folder/118638291458`. The interface includes a search bar, navigation icons, and a sidebar with folder management tools. The main content area displays a list of folders and files under the path `All Files > ... > 2020 > online docs > ☆ ATPESC Attendees`. The list is organized into columns for 'Name' and 'Updated'. The folders listed are Track 0 through Track 8, each updated 'Yesterday by Loy, Raymond M.'. At the bottom of the list is a file named `QUICK REFERENCE.boxnote`, also updated 'Yesterday by Loy, Ra'.

Name ^	Updated
Track 0 - Introduction	Yesterday by Loy, Raymond M.
Track 1 - Hardware Architectures	Yesterday by Loy, Raymond M.
Track 2 - Programming Models and Languages	Yesterday by Loy, Raymond M.
Track 3 - Data Intensive Computing and IO	Yesterday by Loy, Raymond M.
Track 4 - Data Analysis and Visualization	Yesterday by Loy, Raymond M.
Track 5 - Numerical Algorithms and Software	Yesterday by Loy, Raymond M.
Track 6 - Performance Tools and Debuggers	Yesterday by Loy, Raymond M.
Track 7 - Software Productivity	Yesterday by Loy, Raymond M.
Track 8 - Machine Learning	Yesterday by Loy, Raymond M.
QUICK REFERENCE.boxnote	Yesterday by Loy, Ra



anl.app.box.com/notes/695095101259

New

QUICK REFERENCE

Agenda <https://extremecomputingtraining.anl.gov/agenda-2020/>

Zoom Meeting Links

Main Room <---- ALL DAYS WILL START IN THE MAIN ROOM
<https://exascaleproject.zoomgov.com/j/1608499706?pwd=NFhkdlldzZmpjSmRTWWJVVdUkzTGV3Zz09>
Meeting ID: 160 849 9706
Password: 626483

Room B (Used by break-outs as listed in the Agenda)
<https://exascaleproject.zoomgov.com/j/1601131634?pwd=SDRSNETKT3daQ0xqL0FSOC9rMG5yQT09>
Meeting ID: 160 113 1634
Password: 9pgW.M

Room C (Used by break-outs as listed in the Agenda)
<https://exascaleproject.zoomgov.com/j/1610856640?pwd=SHRINKpGWGY2RDFPeUs2SmJRby9nUT09>
Meeting ID: 161 085 6640
Password: 21DRKC

Slack Workspace

<https://alcf-workshops.slack.com>

This Quick Reference Document: <https://anl.app.box.com/notes/695095101259>



ATPESC Slack

- alcf-workshops.slack.com
- #announce
- #general for Q&A during the program
 - There are also topic-related channels
 - See Channels + option to browse the list
- #alcf-account-support ← help with Theta and Cooley accounts
- #atpesc-support ← other logistical help

Getting help

- ALCF accounts (Theta, Cooley)
 - support@alcf.anl.gov and slack #alcf-account-support
- OLCF accounts
 - Token issues, call: 865.241.6536 (24x7). Other questions, email: help@olcf.ornl.gov (mention ATPESC in subject)
- NERSC accounts
 - accounts@nerosc.gov (mention ATPESC in subject) or call 1-800-666-3772
- ATPESC general support including Slack, Box
 - support@extremecomputingtraining.anl.gov
 - #atpesc-support

(**TENTATIVE**) Virtual Argonne National Laboratory Tour

Saturday, August 1 11AM-2PM (expected one hour in this range, watch for updates)

The **Argonne Leadership Computing Facility (ALCF)** is one half of the U.S. Department of Energy's (DOE) Leadership Computing Facility, which deploys diverse high-performance computer architectures that are 10 to 100 times more powerful than typical research computing.



Acknowledgments

Exascale Computing Project



EXASCALE COMPUTING PROJECT

Website: <https://exascaleproject.org>

This training and research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.

ATPESC 2021

- If you or an associate is interested in attending
 - Subscribe to mailing list <https://extremecomputingtraining.anl.gov> (bottom of page)
 - Call for applications usually opens in early January
 - *Read the application instructions carefully*
 - Statement of Purpose and Letter of Recommendation should address how the candidate meets the prerequisites *in detail*.

The future... Aurora Exascale System

